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Letters to the Editor

Surface states of deformed finite crystals

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Various one dimensional models, studied during the last two decades or so (e.g. Davison & Steslicka (1971), Phariseau (1960), Koutecky (1957) have thrown considerable light on the nature of electronic energies of surface states; these models are more realistic than the premier one due to Tamm (1932).

In the present note, we report the derivation of the equation determining the energies of surface states of a finite crystal shown in figure 1. There surface atoms

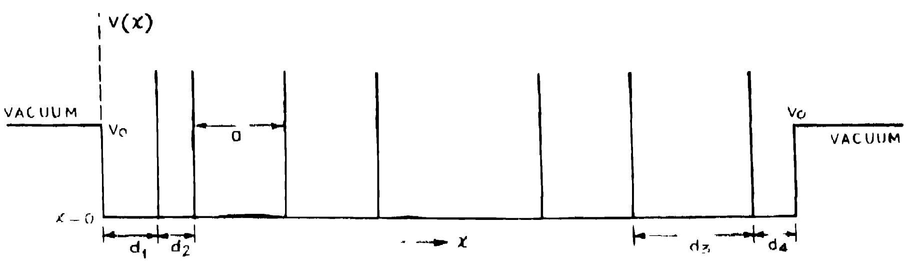

Fig. 1

are assumed to be distorted from their periodic positions; the model thus formulated takes well the care of the experimental findings regarding surface deformations (Davison & Levine 1970). Following the practice in vogue, the atomic potentials are represented by Dirac δ-function of strength :

$$\left(\frac{\hbar^2}{2ma}P\right)$$

To begin with the treatment, we notice that the wavefunctions in various regions appear as given below

$$\psi^1 = A^1 \exp\left[\frac{x}{a}\phi(\zeta)\right], \quad x \leqslant 0 \qquad \ldots (1)$$

$$\psi^2 = A^2 \cos k_1 x + B^2 \sin k_1 x, \quad 0 \leqslant x \leqslant d_1, \qquad \ldots (2)$$

$$\psi^3 = A^3 \cos k_1 x + B^3 \sin k_1 x, \quad d_1 \leqslant x \leqslant d_1 + d_2 \qquad \ldots (3)$$

$$\psi_m = A_m \sin k_1(x-ma) + B_m \sin k_1(a-x-ma), \quad \ldots (4)$$

for, $m = 0, 1 \ldots n$; $ma+d_1+d_2 \leqslant x \leqslant (m+1)a+d_1+d_2$

$$\psi^4 = A^4 \cos k_1 x + B^4 \sin k_1 x; \; na+d_1+d_2 \leqslant x \leqslant d_1+d_2+d_3+na, \ldots \quad \ldots (5)$$

$$\psi^5 = A^5 \cos k_1 x + B^5 \sin k_1 x, \quad \ldots (6)$$

for, $d_1+d_2+d_3+na \leqslant x \leqslant d_1+d_2+d_3+d_4+na$,

$$\psi^6 = A^6 \exp[-\phi(\rho)/a\{x-na-d_1-d_2-d_3-d_4\}], \quad \ldots (7)$$

for, $x > na+d_1+d_2+d_3+d_4$

In the above expressions for the save functions, A's and B's are arbitrary constants. Further

$$k_1 = \frac{1}{\hbar}\sqrt{2mE}, \quad \phi(\rho) = \sqrt{q^2-\zeta^2},$$

$$\rho = ak_1, \quad q = \frac{1}{\hbar}\sqrt{2m(V_0-E)}$$

E = energy of the electron.

The wave functions ψ^1 and ψ^6 are exponentially decaying solutions to the Schrodinger equation with $E < V_0$, for regions outside the crystal. The form of ψ_m is due to Sokolov (1934), also in Steslicka (1973) and it conforms to the validity of Bloch's theorem in the region where the potential is periodic with periodicity a; this region corresponds to the condition : $d_1+d_2 \leqslant x \leqslant na+d_1+d_2$. The constants A_m and B_m are expressible in terms of other two constants C_1 and C_2 :

$$A_m = c_1 \cos \lambda(m+1) + c_2 \sin \lambda(m+1) \quad \ldots (8)$$

$$B_m = c_1 \cos m\lambda + c_2 \sin m\lambda \quad \ldots (9)$$

where,

$$\cos \lambda = \cos \zeta + (P/\zeta) \sin \zeta$$

The remaining wave functions are all solutions to the Schrodinger equation for free electron.

Now, the wave functions (1) to (7) are required to satisfy the following boundary conditions

$$(\psi^1)_{x=0} = (\psi^2)_{x=0} \quad \ldots (10)$$

$$\left(\frac{d\psi^1}{dx}\right)_{x=0} = \left(\frac{d\psi^2}{dx}\right)_{x=0} \quad \ldots (11)$$

$$(\psi^2)_{x=d_1} = (\psi^3)_{x=d_1} \quad \ldots (12)$$

$$\left(\frac{d\psi^2}{dx}\right)_{x=d_1} = \left(\frac{d\psi^3}{dx}\right)_{x=d_1} - (P/\zeta)\psi^3 \quad \ldots \quad (13)$$

$$(\psi^3)_{x=d_1+d_2} = (\psi_0)_{x=d_1+d_2} \quad \ldots \quad (14)$$

$$\left(\frac{d\psi^3}{dx}\right)_{x=d_1+d_2} = \left(\frac{d\psi_0}{dx}\right)_{x=d_1+d_2} - (P/\zeta)\psi_0 \quad \ldots \quad (15)$$

$$(\psi_n)_{x=na+d_1+d_2} = (\psi^4)_{x=na+d_1+d_2} \quad \ldots \quad (16)$$

$$\left(\frac{d\psi_n}{dx}\right)_{x=na+d_1+d_2} = \left(\frac{d\psi^4}{dx}\right)_{x=na+d_1+d_2} - (P/\zeta)\psi^4 \quad \ldots \quad (17)$$

$$(\psi^4)_{x=na+d_1+d_2+d_3} = (\psi^5)_{x=na+d_1+d_2+d_3} \quad \ldots \quad (18)$$

$$\left(\frac{d\psi^4}{dx}\right)_{x=na+d_1+d_2+d_3} = \left(\frac{d\psi^5}{dx}\right)_{x=na+d_1+d_2+d_3} - (P/\zeta)\psi^5 \quad \ldots \quad (19)$$

$$(\psi^5)_{x=na+d_1+d_2+d_3+d_4} = (\psi^6)_{x=na+d_1+d_2+d_3+d_4} \quad \ldots \quad (20)$$

$$\left(\frac{d\psi^5}{dx}\right)_{x=na+d_1+d_2+d_3+d_4} = \left(\frac{d\psi^6}{dx}\right)_{x=na+d_1+d_2+d_3+d_4} \quad \ldots \quad (21)$$

Restoring the wavefunctions (1) to (7) in the boundary conditions (10) to (21), we get a system of twelve equations involving fourteen constants : A^1 to A^6, B^2 to B^5, A_0, B_0, A_n, B_n. These twelve equations can be combined so as to obtain finally the following two equations in terms of the constants C_1 and C_2

$$C_1T_0 - C_2T_2 = 0 \quad \ldots \quad (22)$$

$$C_1T_3 - C_2T_4 = 0 \quad \ldots \quad (23)$$

Eq. (22) corresponds to a combination of (10) to (15) while (23) is the result of grouping of (16) to (21). The expressions for T_0 to T_4, as well as the forms of other entities on which they depend, are given below :

$$T_0 = F_2 - \cos\lambda \quad \ldots \quad (24)$$

$$T_2 = F_1 \sin\lambda \quad \ldots \quad (25)$$

$$T_3 = F_3 \cos\lambda(n+1) \quad \ldots \quad (26)$$

$$T_4 = F_4 \sin n\lambda - F_3 \sin\lambda(n+1) \quad \ldots \quad (27)$$

$$F_1 = f_7 - \left(\frac{\phi}{\zeta}\right) f_5 \tag{28}$$

$$F_2 = \left(\frac{\phi}{\zeta}\right) f_6 - f_8 \tag{29}$$

$$F_3 = f_{13} f_{17} - f_{15} f_{18} \tag{30}$$

$$F_4 = f_{16} f_{18} - f_{14} f_{18} \tag{31}$$

$$f_1 = \frac{r}{\zeta} \sin^2 \zeta(\delta_2 + \delta_1) \tag{32}$$

$$f_2 = \sin \zeta + \frac{r}{\zeta} \sin \zeta(\delta_1 + \delta_2) \sin \zeta(1 - \delta_1 - \delta_2) \quad \ldots \tag{33}$$

$$f_3 = \sin \zeta(\delta_2 + \delta_1) - f_1 \cos \zeta(\delta_2 + \delta_1) \quad \ldots \tag{34}$$

$$f_4 = \sin \zeta(1 - \delta_2 - \delta_1) - f_2 \cos \zeta(\delta_2 + \delta_1) \quad \ldots \tag{35}$$

$$f_5 = f_1 \left(1 + \frac{P}{\zeta} \cos^2 \zeta\delta_1\right) + \frac{P}{\zeta} f_3 \sin^2 \zeta\delta_1 \quad \ldots \tag{36}$$

$$f_6 = f_2(1 + (P/\zeta)\cos^2\zeta\delta_1) + (P/\zeta) f_4 \sin^2 \zeta\delta_1 \quad \ldots \tag{37}$$

$$f_7 = f_1 \cot \zeta\delta_1 + f_3 - f_3 \cot \zeta\delta_1 \quad \ldots \tag{38}$$

$$f_9 = \sin(n\zeta) - (P/\zeta) \sin \zeta(1 - \delta_1 - \delta_2) \quad \ldots \tag{39}$$

$$f_{10} = \sin(n\zeta) - (P/\zeta) \sin \zeta(1 - \delta_1 - \delta_2) \sin \zeta(n + \delta_1 + \delta_2) \quad \ldots \tag{40}$$

$$f_{11} = \{\sin \zeta(n + \delta_1 + \delta_2)\}^{-1} \{\sin \zeta(\delta_1 + \delta_2) - f_9\} \quad \ldots \tag{41}$$

$$f_{12} = \{\sin \zeta(n + \delta_1 + \delta_2)\}^{-1} \{\sin \zeta(1 - \delta_1 - \delta_2) - f_{10}\} \quad \ldots \tag{42}$$

$$f_{13} = f_9[1 - (P/\zeta) \sin \zeta(n + \delta_1 + \delta_2 + \delta_3)] - (P/\zeta) f_{11} \sin^2 \zeta(n + \delta_1 + \delta_2 + \delta_3) \quad \ldots \tag{43}$$

$$f_{14} = f_{10} \left[1 - \left(\frac{P}{\zeta}\right) \sin \zeta(n + \delta_1 + \delta_2 + \delta_3)\right] - \left(\frac{P}{\zeta}\right) f_{12} \sin^2 \zeta(n + \delta_1 + \delta_2 + \delta_3) \quad \ldots \tag{44}$$

$$f_{15} = \{\sin \zeta(n + \delta_1 + \delta_2 + \delta_3)\}^{-1} \{f_9 \cos \zeta(n + \delta_1 + \delta_2 + \delta_3) + f_{11} \sin \zeta(n + \delta_0 + \delta_2 + \delta_3) - f_{13} \cos \zeta(n + \delta_0 + \delta_2 + \delta_3)\} \quad \ldots \tag{45}$$

$$f_{16} = \{\sin \zeta(n + \delta_0 + \delta_2 + \delta_3)\}^{-1} \{f_{10} \cos \zeta(n + \delta_0 + \delta_2 + \delta_3) + f_{12} \sin \zeta(n + \delta_0 + \delta_2 + \delta_3) - f_{14} \cos \zeta(n + \delta_0 + \delta_2 + \delta_3)\} \quad \ldots \tag{46}$$

$$f_8 = f_4 - f_6 \cot(\zeta\delta_1) \quad \ldots \text{(47}$$

$$f_{17} = \cos\zeta(n+\delta_1+\delta_2+\delta_3)-\frac{\phi(\zeta)}{\zeta}\sin\zeta\,(n+\delta_1+\delta_2+\delta_3) \quad \ldots \quad (48)$$

$$f_{18} = -\cos\zeta(n+\delta_1+\delta_2+\delta_3)-\frac{\phi(\zeta)}{\zeta}\sin\zeta\,(n+\delta_1+\delta_2+\delta_3)\,\cdot \quad \ldots \quad (49)$$

$$\delta_i = \frac{d_i}{a}, \quad i = 1, 2, 3, 4.$$

Now, in order that (22) and (23) yield non zero solutions for C_1 and C_2, the following equation must hold good

$$T_4T_4 - T_2T_3 = 0 \quad \ldots \quad (50)$$

Taking λ to be complex and solving (50) for ζ, we can obtain the energies of surface states via the relation $\zeta = a/\hbar\sqrt{2mE}$. It may be mentioned here that the objective behind the studies of one dimensional models by several other authors (e.g. Davison & Stoslicka (1971), Koutecky (1957) is to derive equations analogous to (50). A comparison of the energy spectrum on the basis of (50) with the ones of the afore-mentioned works will bring out the extent of quantitative importance of the special features of our model. These aspects, together with the relevant numerical analysis of (50), would be discussed in a future communication.

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